SAND REPORT

SAND2004-4834
Unlimited Release
Printed October 2004

Damage Displacement Phenomena in Si Juction Devices: Mapping and Interpreting a Science and Technology Knowledge Domain

J. Y. Tsao

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia is a multiprogram laboratory operated by Sandia Corporation,
a Lockheed Martin Company, for the United States Department of
Energy under Contract DE-AC04-94AL85000.

Approved for public release; further dissemination unlimited.

Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.
NOTICE: This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865)576-8401
Facsimile: (865)576-5728
E-Mail: reports@adonis.osti.gov
Online ordering: http://www.doe.gov/bridge

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd
Springfield, VA 22161

Telephone: (800)553-6847
Facsimile: (703)605-6900
E-Mail: orders@ntis.fedworld.gov
Online order: http://www.ntis.gov/ordering.htm

SAND2004-4834
UNLIMITED RELEASE
PRINTED OCTOBER 2004

Damage Displacement Phenomena in Si Junction Devices: Mapping and Interpreting a Science and Technology Knowledge Domain

J. Y. Tsao
Semiconductor Material and Device Sciences Department

Sandia National Laboratories
P. O. Box 5800, Albuquerque, NM 87185

Abstract

As technical knowledge grows deeper, broader, and more interconnected, knowledge domains increasingly combine a number of sub-domains. More often than not, each of these sub-domains has its own community of specialists and forums for interaction. Hence, from a generalist's viewpoint, it is sometimes difficult to understand the relationships between the sub-domains within the larger domain; and, from a specialist's viewpoint, it may be difficult for those working in one sub-domain to keep abreast of knowledge gained in another sub-domain. These difficulties can be especially important in the initial stages of creating new projects aimed at adding knowledge either at the domain or sub-domain level.

To circumvent these difficulties, one would ideally like to create a map of the knowledge domain – a map which would help clarify relationships between the various sub-domains, and a map which would help inform choices regarding investing in the production of knowledge either at the domain or sub-domain levels.

In practice, creating such a map is non-trivial. First, relationships between knowledge sub-domains are complex, and not likely to be easily simplified into a visualizable 2-or-few-dimensional map. Second, even if some of the relationships can be simplified, capturing them would require some degree of expert understanding of the knowledge domain, rendering impossible any fully automated method for creating the map.

In this work, we accept these limitations, and within them, attempt to explore semi-automated methodologies for creating such a map.

We chose as the knowledge domain for this case study "displacement damage phenomena in Si junction devices." This knowledge domain spans a particularly wide range of knowledge sub-domains, and hence is a particularly challenging one.

It is also a knowledge domain of current interest, at Sandia and worldwide. In a number of applications, including space electronics, high-energy physics experimentation, and nuclear weaponry, Si junction devices will be exposed, either continuously or in bursts, to high-energy particles. These particles displace atoms in the Si lattice, creating defects. The defects, in turn, have properties which influence the electronic behavior of the devices. They also have properties which influence how they diffuse and react with other defects in the lattice, and ultimately influence the short- and long-term evolution of the electronic behavior of the devices.

Intentionally left blank

Contents

Introduction 6
Building the Knowledge Domain 7
Organize the Knowledge Domain into Classes spanning a range of Time and Spatial Scales 8
New "Exogenous" Mapping Technique 10
Keyword and Training Sets 12
Time-Space Map of Displacement Damage Phenomena (DDP) 13
Foundational DPP Knowledge 15
Projected Cites and Emerging DPP Knowledge 16
Emerging DPP Knowledge 17
"Missing" DPP Knowledge 18
Distribution 19

Displacement Damage Phenomena (DDP) in Si Junction Devices

Mapping and interpreting a science and technology knowledge domain

Acknowledgements:
Kevin Horn, Kevin Boyack, Nabeel Rahal, Wendland Beezhold

Sandia National Laboratories

1. As technical knowledge grows deeper, broader, and more interconnected, knowledge domains increasingly combine a number of sub-domains. More often than not, each of these sub-domains has its own community of specialists and forums for interaction. Hence, from a generalist's viewpoint, it is sometimes difficult to understand the relationships between the sub-domains within the larger domain; and, from a specialist's viewpoint, it may be difficult for those working in one sub-domain to keep abreast of knowledge gained in another sub-domain. These difficulties can be especially important in the initial stages of creating new projects aimed at adding knowledge either at the domain or sub-domain level.
2. To circumvent these difficulties, one would ideally like to create a *map* of the knowledge domain – a map which would help clarify relationships between the various sub-domains, and a map which would help inform choices regarding investing in the production of knowledge either at the domain or sub-domain levels.
3. In practice, creating such a map is non-trivial. First, relationships between knowledge sub-domains are complex, and not likely to be easily simplified into a visualizable 2-or-few-dimensional map. Second, even if some of the relationships can be simplified, capturing them would require some degree of expert understanding of the knowledge domain, rendering impossible any fully automated method for creating the map.
4. In this work, we accept these limitations, and within them, attempt to explore semi-automated methodologies for creating such a map.
5. We chose as the knowledge domain for this case study "displacement damage phenomena in Si junction devices." This knowledge domain spans a particularly wide range of knowledge sub-domains, and hence is a particularly challenging one.
6. It is also a knowledge domain of current interest, at Sandia and worldwide. In a number of applications, including space electronics, high-energy physics experimentation, and nuclear weaponry, Si junction devices will be exposed, either continuously or in bursts, to high-energy particles. These particles displace atoms in the Si lattice, creating defects. The defects, in turn, have properties which influence the electronic behavior of the devices. They also have properties which influence how they diffuse and react with other defects in the lattice, and ultimately influence the short- and long-term *evolution* of the electronic behavior of the devices.

Building the Knowledge Domain

1
- Search for articles with key words: Displacement <and> Damage <and> (Silicon <or> Device)
- Dump to Procite
- Cull articles outside of knowledge domain, using keywords such as GaAs <or> InP <or> CCD <or> Oxide <or> Carbide <or> FET <or> MOS

2
- Forward and backward citation expansion around most-highly-cited articles
- Cull articles outside of knowledge domain

Jeff Tsao • Mapping/Interpreting Damage Displacement Phenomena • 2004 Sep 9

Sandia National Laboratories

1. To start, we built a representation of the knowledge domain from the technical literature. We note at the outset that such a representation cannot be a complete one. The technical literature represents only that part of the knowledge domain that has been "codified," and neglects that part that is "tacit", existing only in people -- their experiences and how they go about doing things. This is perhaps less so in science, perhaps more so in engineering, but it is always represents an omission of some kind.
2. Nevertheless, with this as a caveat, we built a representation of the "codified" knowledge domain using the technical literature. We used the 2-step sequence illustrated in this slide.
3. First, we searched the Institute for Scientific Information (ISI) database for articles containing key words associated with damage displacement phenomena in silicon materials or devices. These articles were dumped into a Procite database (Procite is a standard bibliographic database program used by Sandia's librarians). Articles outside of the knowledge domain were manually culled through use of key words such as GaAs, InP, CCD, Oxide, Carbide, FET or MOS.
4. Second, forward and backward citation "expansions" were done around the most highly-cited articles: all articles which either cited, or were cited by, these highly-cited articles were added to the database. Then, another round of manual culling was done. This cycle was repeated several times, until ultimately the database contained approximately 650 articles.
5. Note that even these 650 articles aren't a comprehensive representation of even the codified part of the knowledge domain. If we wanted comprehensiveness, we would have repeated the citation expansion cycle 2 several more times until we found the database saturating in size. And, we would have added additional cycles involving searching for articles written by highly-cited authors or author pairs, again, until we found the database saturating in size.
6. However, through our use of at least several iterations of the citation expansion step 2, we think the database at least contains most of the important articles in the knowledge domain (this was checked at an informal level by Wendland Beezhold (15341), a researcher in this knowledge domain).

Organize the Knowledge Domain into Classes spanning a range of Time and Spatial Scales

Increasing Time Scale

	Class	Time Scale (s)	Space Scale (m)
A	Nuclear Scattering and Reactions	10^{-19}	10^{-13}
B	Nuclear Displacements and Carrier Ionization	10^{-14}	10^{-9}
C1	Defects and Disorder	10^{-12}	10^{-8}
C2	Irradiated Materials	10^{-12}	10^{-8}
D1	Irradiated Diode Particle Detectors	10^{-8}	10^{-5}
D2	Irradiated Photo detectors and Solar Cells	10^{-8}	10^{-5}
D3	Irradiated Diodes	10^{-8}	10^{-5}
D4	Irradiated Transistors and other Devices	10^{-8}	10^{-5}
E	Irradiated Circuits and System Applications	10^{-6}	10^{-3}
F	Defect Interactions and Materials Annealing	10^{-3}	10^{-8}
G	Device Annealing	10^{-3}	10^{-5}

Jeff Tsao • Mapping/Interpreting Damage Displacement Phenomena • 2004 Sep 9

Sandia National Laboratories

1. Now, because we want to create a map of this database, and we want this map to be organized in a physically meaningful way, our next step was to classify the articles according to the physical phenomena discussed in the article. There must certainly be many ways of doing such classifying, depending on the types of physical phenomena that one is attuned to. However, the classes that emerged seemed relatively "obvious," and we suspect others with some understanding of this knowledge domain would have classified the articles similarly, or would at least view our classes as reasonable. The seven overall classes are listed in this slide, organized roughly according to the time and spatial scales associated with the phenomena studied in those classes.
2. At the shortest time scale, in white, is direct nuclear scattering and reaction. Its time scale varies over a range, depending on whether it is scattering or reaction we are talking about. But for a 0.001-1 MeV neutron with velocity $v \sim (0.01\text{MeV}/1\text{GeV})^{0.5}c \sim 10^6$ m/s incident on a lattice nucleus of dimension 10^{-13} m, the time and space scales of a scattering event would be on the order of $dt \sim dx/v \sim 10^{-19}$ s and $dx \sim 10^{-13}$ m.
3. At just longer time scales, in yellow, is nuclear displacement and carrier ionization. Its time and space scales also vary over a range, depending on the energy of the incident particle. But for a near-end-of-range 100 eV neutron with velocity $v \sim (100\text{eV}/1\text{GeV})^{0.5}c \sim 10^5$ m/s incident on a lattice site of dimension 10^{-9} m, the time and space scales of nuclear displacements would be on the order of $dt \sim dx/v \sim 10^{-14}$ s and $dx \sim 10^{-9}$ m.
4. At just longer time scales, in purple, are defects and irradiated materials. These could be broken down into two sub-classes (defects and disorder, and irradiated materials), but for our purpose here we lump them together into one class related to the response of those defects and materials to the electronic phenomena occurring in a device. Hence, the time and space scales associated with this class are those associated with carrier scattering and trapping by lattice defects. To give these scales orders of magnitude, for a carrier incident at a typical drift velocity ($v \sim 10^4$ m/s) on a defect with a hydrogen-atom-like Bohr radius ($r \sim 10^{-8}$ m), the time and space scales would be on the order of 10^{-12} s and 10^{-8} m, respectively.

Organize the Knowledge Domain into Classes spanning a range of Time and Spatial Scales

Increasing Time Scale

	Class	Time Scale (s)	Space Scale (m)
A	Nuclear Scattering and Reactions	10^{-19}	10^{-13}
B	Nuclear Displacements and Carrier Ionization	10^{-14}	10^{-9}
C1	Defects and Disorder	10^{-12}	10^{-8}
C2	Irradiated Materials	10^{-12}	10^{-8}
D1	Irradiated Diode Particle Detectors	10^{-8}	10^{-5}
D2	Irradiated Photo detectors and Solar Cells	10^{-8}	10^{-5}
D3	Irradiated Diodes	10^{-8}	10^{-5}
D4	Irradiated Transistors and other Devices	10^{-8}	10^{-5}
E	Irradiated Circuits and System Applications	10^{-6}	10^{-3}
F	Defect Interactions and Materials Annealing	10^{-3}	10^{-8}
G	Device Annealing	10^{-3}	10^{-5}

Jeff Tsao • Mapping/Interpreting Damage Displacement Phenomena • 2004 Sep 9

Sandia National Laboratories

1. At just longer time scales yet, in green, are irradiated devices. These can be broken down into the four sub-classes indicated, but for our purpose here we lump them together into one class related to the response of internal currents and voltages in the device to externally imposed currents and voltages. Since this knowledge domain is restricted to p-n junction devices, we consider a typical depletion length of $l \sim 10^{-5}$ m and a typical drift time through that depletion length of $t \sim 10^{-8}$ s.
2. At just longer time scales yet, in red, are irradiated circuits and system applications. Here we are concerned with circuit phenomena, whose time and space scales are roughly 10-100x longer and larger than those for devices. Hence, we associate these phenomena with time and space scales of roughly $l \sim 10^{-3}$ m and $t \sim 10^{-6}$ s.
3. Finally, at the longest time scales, we have phenomena associated with annealing. Defect interactions and materials annealing is in orange, and device annealing is in black. The time scale for such annealing covers an extremely wide range. For our purpose we associate this phenomena with a time scale on the order of 10^{-3} s, a time scale intermediate between the short-term annealing that may occur during the process of defect creation itself and the very long-term annealing that occurs over the potentially many-years' lifespan of the device. For their space scales we associate the same space scales used for defects and irradiated materials (10^{-8} m) and devices (10^{-5} m).
4. Note that in discussing the phenomena associated with these seven classes, it was natural to distinguish them according to their time and space scales. There may be other ways to distinguish them that are just as natural. However, in what follows, we attempt to use these axes, time and space scales, to map the articles in the database.

New "Exogenous" Mapping Technique

1-2b Keyword popularity = Number of times n_i keyword i appears in any title or class

1-2a Number of times n_{ik} keyword i appears in class k

1-3 Keyword weights = information content: $w_i = \sum_k (n_{ik}/n_i)\ln(n_{ik}/n_i) - \ln(1/\sum_k 1)$

1-4 Choose keywords i that maximize information content and popularity product $I_i = w_i n_i$

2-3 Vary keyword coordinates (x_i, y_i) to minimize

$$\delta^2 = \delta x^2 + \delta y^2 = \sum_{j \in D_\alpha} \left[(x_j^a - x_j^m)^2 + (y_j^a - y_j^m)^2 \right]$$

2-1 Baseline coordinates are time and spatial scale of class

Keyword	n_i	n_{iG}	n_{iF}	n_{iE}	n_{iD4}	n_{iD3}	n_{iD2}	n_{iD1}	n_{iC2}	n_{iC1}	n_{iB}	n_{iA}	w_i	I_i	x_i	y_i
detect	179	19	3	26	0	3	125	0	0	1	2	0	14	2528	-4.0	-1.4
anneal	59	30	29	0	0	0	0	0	0	0	0	0	17	1005	9.0	-6.8
silicon	384	30	35	25	13	9	107	30	48	58	28	1	3	1125	-6.5	-6.5
diode	77	7	0	10	0	14	3	41	0	2	0	0	10	806	-1.0	0.7
damage	149	7	7	6	16	6	37	37	17	6	37	0	4	539	-18.5	-10.9
displace	44	0	0	7	7	0	0	2	0	0	34	0	17	738	-15.6	-9.6
rad	384	27	26	42	29	20	102	38	37	45	17	1	2	870	-10.9	-8.2
irradiated	144	17	12	1	5	4	37	19	17	30	2	0	4	623	-14.6	-6.8
device	43	7	0	2	28	1	1	0	1	0	3	0	12	529	-3.7	-1.4
defect	91	9	17	2	4	1	14	4	0	38	2	0	7	647	-8.0	-9.3
ion	437	26	35	50	36	20	94	33	37	50	37	45	11	540	-6.7	-3.9
radiation	243	11	14	39	23	15	66	22	20	18	14	1	2	602	-6.7	-4.1

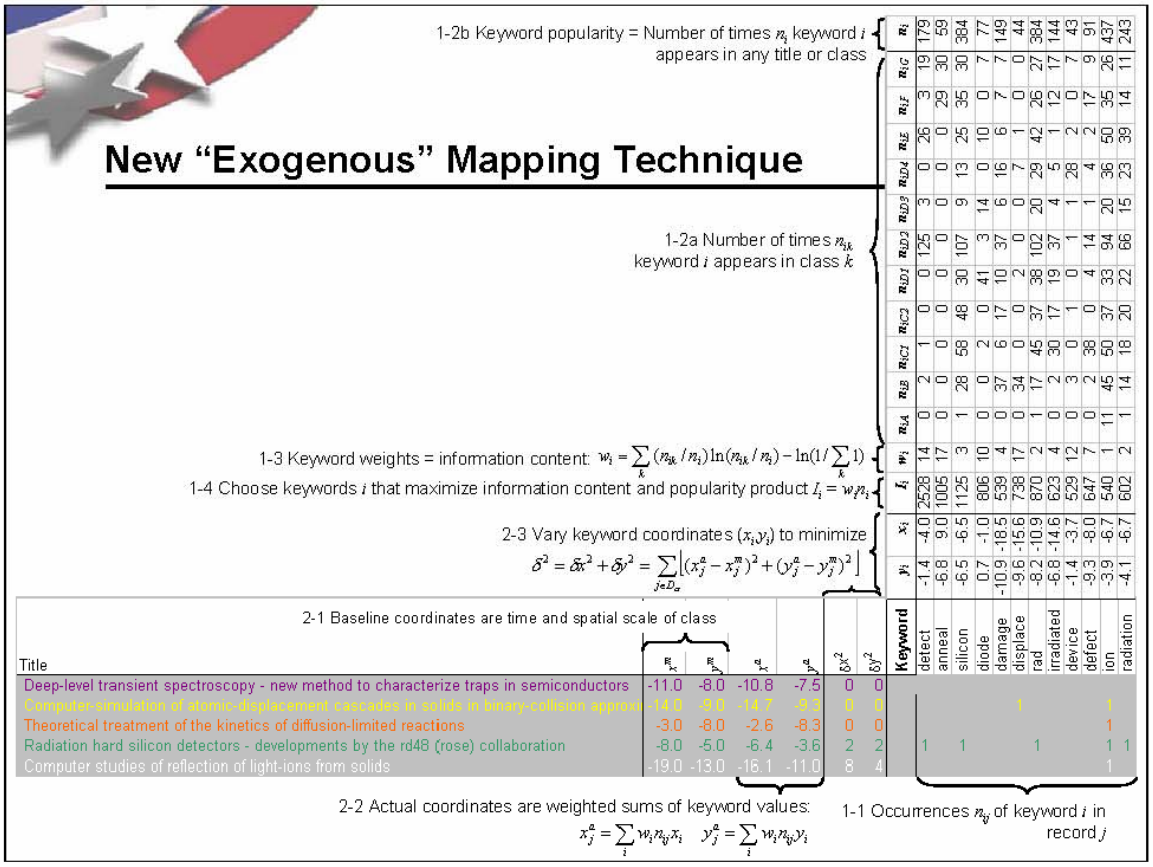
Title	x_j^m	y_j^m	x_j^a	y_j^a	δx_j^2	δy_j^2	detect	anneal	silicon	diode	damage	displace	rad	irradiated	device	defect	ion	radiation
Deep-level transient spectroscopy - new method to characterize traps in semiconductors	-11.0	-8.0	-10.8	-7.5	0	0												
Computer-simulation of atomic-displacement cascades in solids in binary-collision approxi	-14.0	-9.0	-14.7	-9.3	0	0						1						
Theoretical treatment of the kinetics of diffusion-limited reactions	-3.0	-8.0	-2.6	-8.3	0	0										1		
Radiation hard silicon detectors - developments by the rd48 (rose) collaboration	-8.0	-5.0	-6.4	-3.6	2	2	1		1				1				1	1
Computer studies of reflection of light-ions from solids	-19.0	-13.0	-16.1	-11.0	8	4											1	

2-2 Actual coordinates are weighted sums of keyword values:

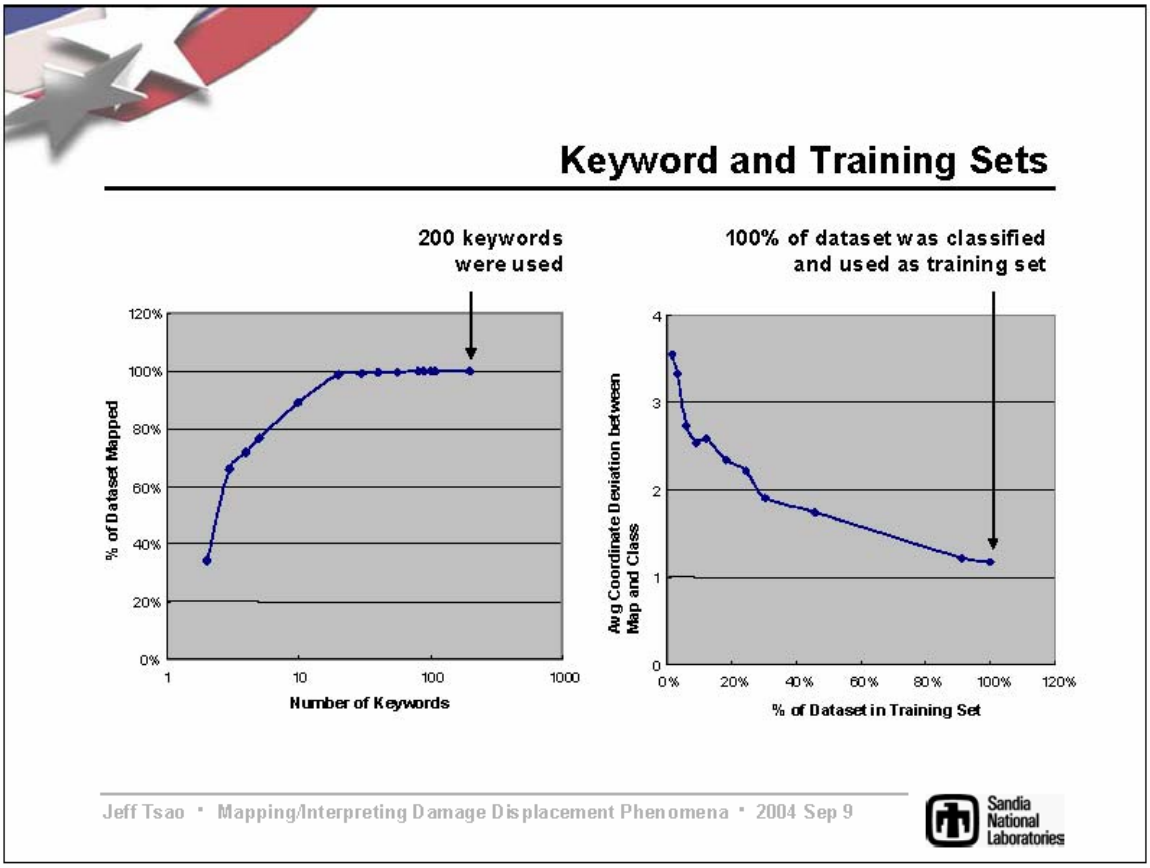
$$x_j^a = \sum_i w_i n_{ij} x_i \quad y_j^a = \sum_i w_i n_{ij} y_i$$

1-1 Occurrences n_{ij} of keyword i in record j

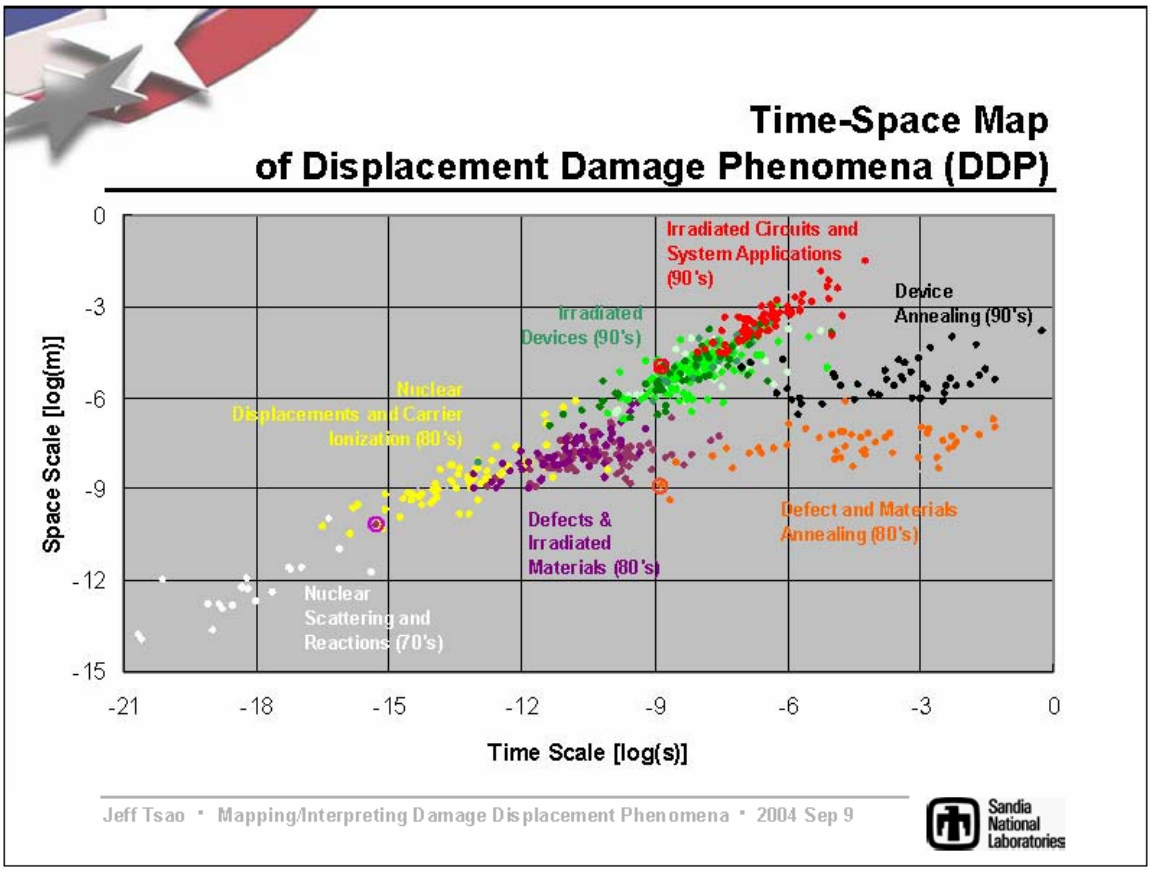
1. In other words, what we'd like to do is map the various articles according to the time and space scales of the phenomena they discuss. In a sense, we have already done this, by grouping the articles into classes, and by associating the classes with particular time and space scales. However, not all articles will be completely in one class – some will have components in other classes, and we'd like to enable these to drift accordingly. And, as they drift, they may enable "mis-classed" articles to emerge.
2. Hence, what we'd like to do is develop a technique for mapping the articles such that we include in a rough way information about the class that the article has been manually classified into, but that allows the positioning of the article to drift according to its lexical content. The technique we developed for doing this is illustrated in this spreadsheet.
3. We start with a column of titles of the articles. It would have been best to use the abstracts for the articles, but for many of the older articles, abstracts weren't readily available, so to be consistent we just used titles. We also start with a row of keywords taken from the titles of the articles. The basic idea is to assign x and y coordinates to those keywords, and then to determine x and y coordinates for each of the articles by calculating the weighted sum of the coordinates of the keywords that appear in the titles of those articles. This idea originated with Kevin Boyack (Org. 09212). The two tricky pieces are: how do we choose the best keywords, and how do we assign x and y coordinates to those keywords?
4. We choose keywords based on the following procedure. First, we calculate the occurrences of our starting set of keywords in all the article titles. Those are the numbers in the intersections of the title rows and keyword columns. A "1" means the keyword appears in the article title, a "0" means it doesn't. Second, we calculate the number of occurrences of our starting set of keywords in the various classes of articles. Those are the numbers in this matrix up here. This "125" means that the keyword "defect" appeared in 125 articles in class D2; this "0" means that it appeared in none of the articles in class D1. We also calculate the overall popularity of the keyword – the number of times the keyword appears in all titles and classes. Third, we calculate the information content of the keywords. Basically, if a keyword is represented equally across the classes, then it has lower information content, but if it is represented unequally across the classes, then it has higher information content. This formula here actually looks a bit like the entropy of a multi-component solution; that's because information content is in a way the inverse of entropy content. Fourth, we calculate the product of that information content of the keyword with its popularity, and use that product to choose keywords. In other words, we want keywords that have high information content, but we also want keywords that are represented in a lot of article titles, so that we don't need as many keywords. In practice, we ended up using 200 keywords, out of an initial set of about 1100 determined by Nabeel Rahal (Org. 05925) using a commercial lexical analysis software program called ClearForest (http://www.clearforest.com/). These are some of the keywords – the ones with the highest information content and popularity product. Detect, anneal and silicon are the highest ranking keywords.



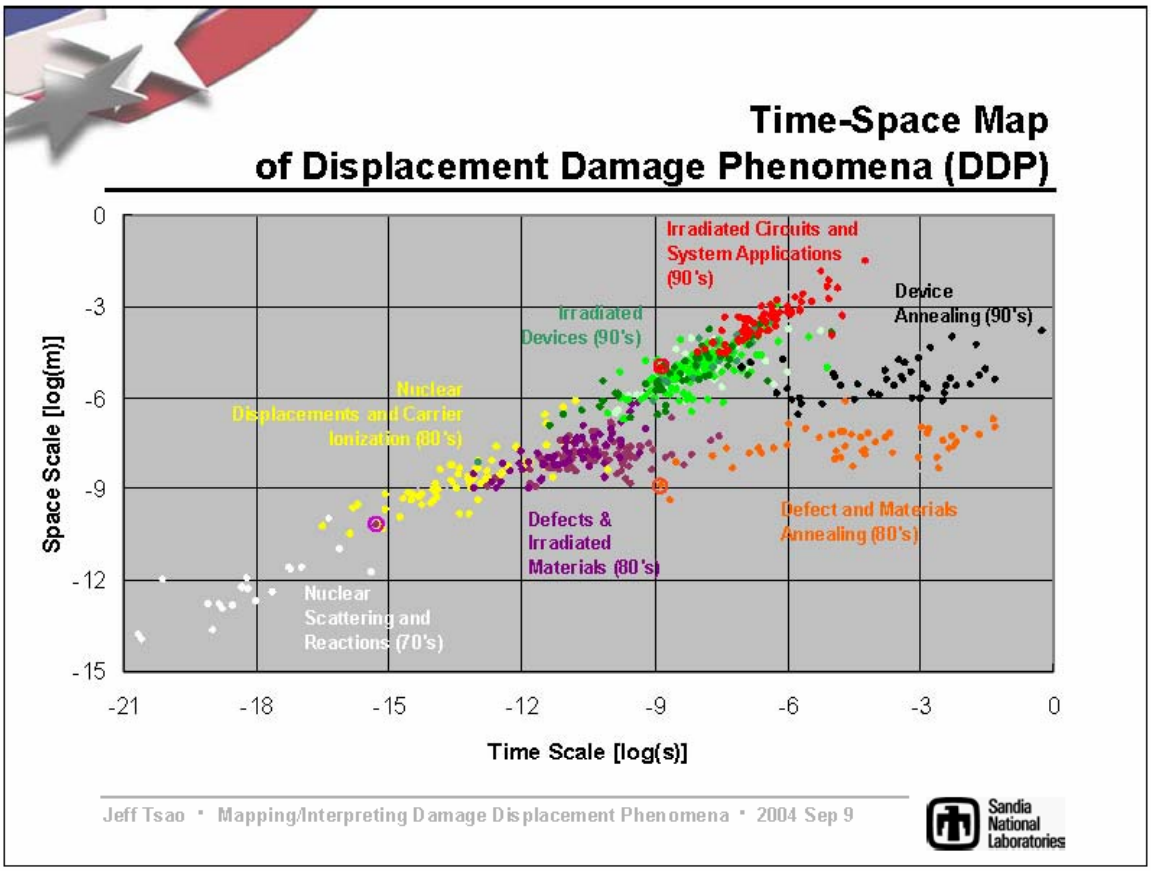
1. Having chosen keywords, now we must assign x and y coordinates to those keywords. We do that using the following procedure. First, we assign baseline x and y coordinates to a subset of the articles – a training set, so to speak. The coordinates we assign are simply the x and y coordinates already assigned to the class that the article was grouped into. Second, we assign an initial set of x and y coordinates to the keywords, and use those coordinates to determine the coordinates of the individual articles themselves, through the weighted sum of the coordinates of the keywords that appear in the titles of those articles. Third, we calculate, for the training set, the sum of the deviations of those keyword-determined coordinates with the class-determined baseline coordinates, and vary the keyword coordinates to minimize that sum. In practice, we ended up using the entire dataset as the training set, since we had already classified every article.
2. So now we have both the keyword weights and the keyword coordinates, and can now assign all of the articles in the database coordinates on a time and space map.



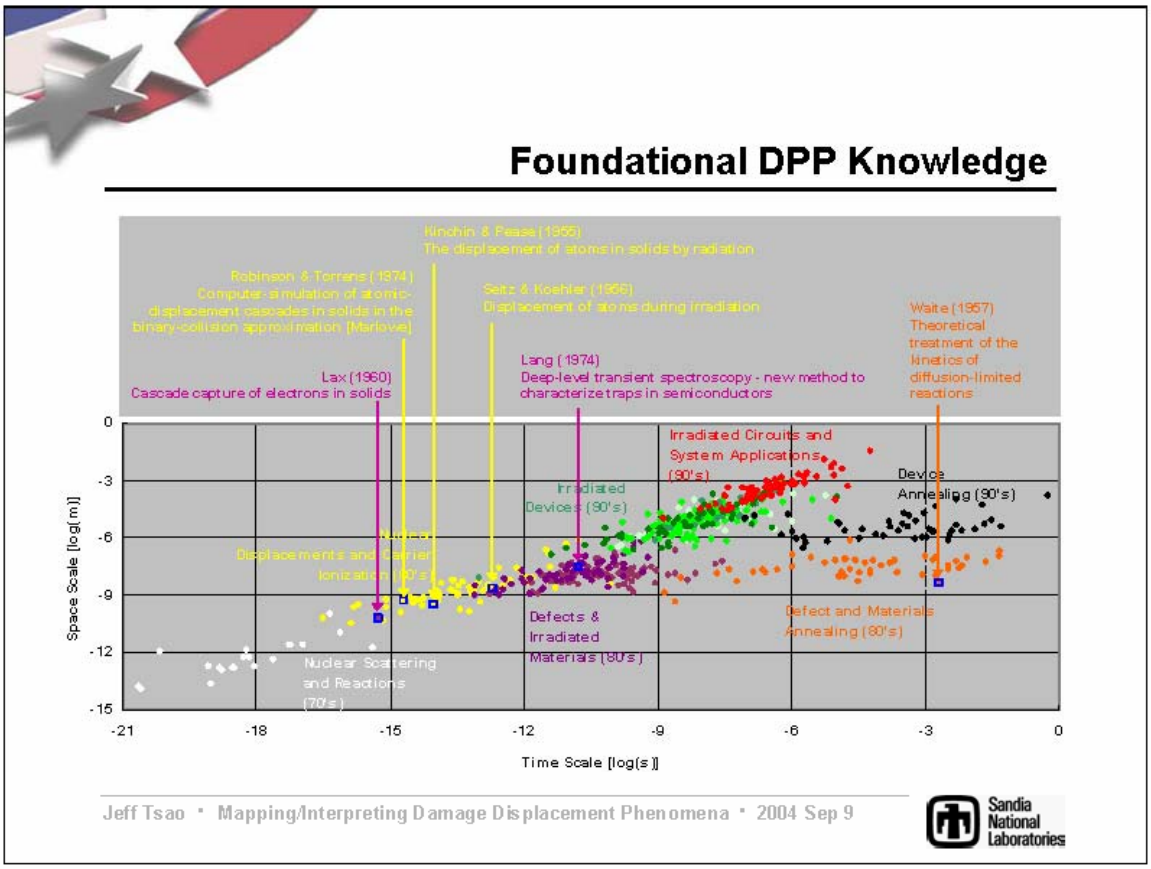
1. But before we do that, here are a couple of minor side-points regarding the mapping methodology we just outlined.
2. The first has to do with the choice of number of keywords to use. As we mentioned, the more keywords that are used, the more likely every article will be represented by one of them. That's illustrated in the left figure, which shows the percentage of articles in the dataset that are mapped rising with the number of keywords used. Once the number of keywords is greater than 50 or so, pretty much every article is represented. However, in practice, the quality of the mapping still improves as the number of keywords increases, because articles are more and more likely to contain more than one keyword. So for the maps we'll show in a minute, we ended up using 200 keywords, very near the maximum number of columns (256) allowed by Excel.
3. The second has to do with the choice of how large to make the training set. The training set is the set of articles that has been "preclassified," and whose mapped coordinates we attempt to align with the coordinates assigned to the classes. The larger the training set, of course, the better able we are to assign coordinates to the keywords. In fact, as shown in the right figure, as the % of the dataset in the training set increases, the deviation between the coordinates resulting from the automated mapping and the coordinates of the classes decreases steadily. Since in this case, we preclassified every article in the dataset, there was no reason not to use the entire dataset as our training set, so that's what we've done in the maps we'll show in a minute.



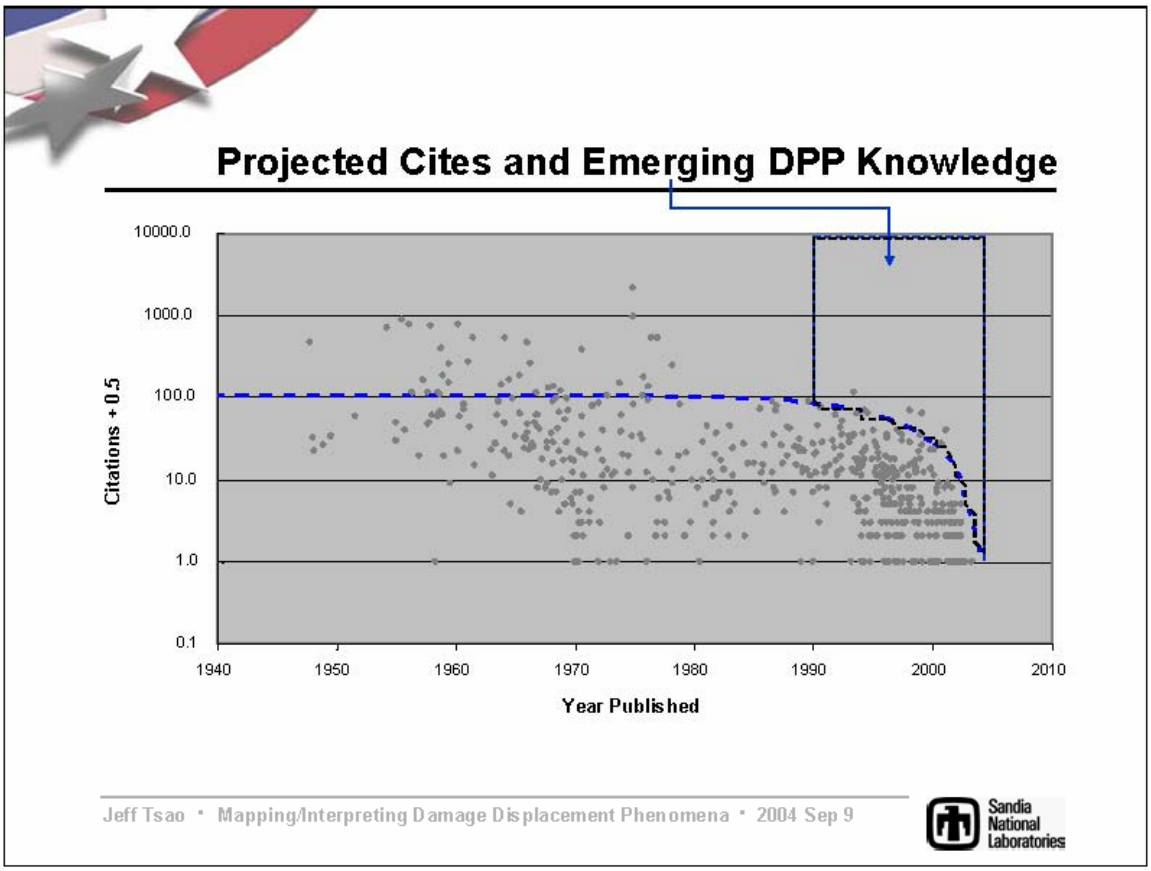
1. The resulting map is shown here. Each dot represents one article, colored according to the class it belongs to. One can see that there is a correlated progression from short times and short spatial scales to long times and long spatial scales, as the phenomena studied shift from nuclear phenomena, to atomic phenomena, to electronic phenomena.
2. At longer times, the classes fan-out into two spatial scales. One is for defects and irradiated materials, where at shorter times one is concerned with electronic properties and how those properties influence device performance, and at longer times one is concerned with their atomic properties and how those properties influence their atomic motion, reaction, and statistical evolution. The other is for irradiated devices, where at shorter times one is concerned with electronic properties with an un-evolved statistical distribution of defects, but at longer times concerned with electronic properties with an evolved statistical distribution of defects.
3. Note that there is a fair amount of dispersion to the mapping – the articles don't cluster tightly around the time and space coordinates associated with their class. Many of the articles are actually mapped into neighboring classes.
4. Some of these are mapping mistakes. This purple dot, e.g., has to do with "cascade capture of electrons in solids." It gets mapped into the nuclear displacements class mainly because cascade is a word more commonly associated with atomic displacements rather than electron capture. And this red dot, e.g., has to do with "radiation hardness of silicon detectors for future colliders." It gets mapped into the irradiated devices class mainly because colliders is a rarely enough used word that it didn't even make it into our keyword list, and hence couldn't be used to give that article more weighting in the irradiated circuits and system applications class.



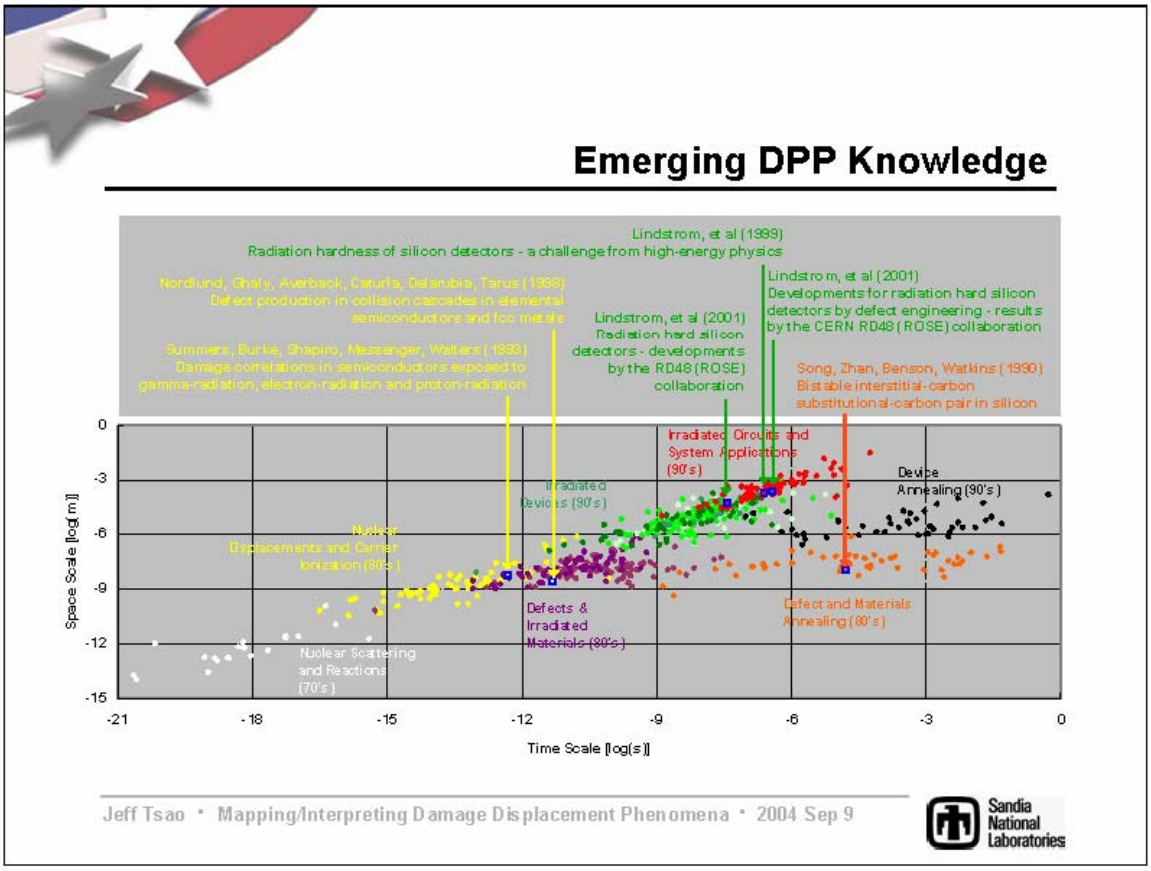
1. But many of them reflect a genuine diversity of phenomena. This orange dot, e.g., has to do with a "model of the charge dependence of formation reactions of radiation defect accumulations in semiconductors." Because formation reactions are the elementary steps associated with annealing, we classified it into the defect and materials annealing class. However, because the charge dependences of those reactions are related tightly to the electronic properties of defects, it drifted fairly close to the defects and irradiated materials class.
2. To give a feeling for the chronology associated with this knowledge domain, we also show on this figure the average decade during which the articles in each class were published.
3. The oldest area is nuclear scattering and reactions, with most of the work published in the 70's. It can be viewed as the most mature of the classes, where thinking has coalesced around established, foundational paradigms.
4. The middle areas are those at slightly longer time and space scales, all having something to do with atomic defects: their creation, properties and evolution. Much of this work was published in the '80's. It can be viewed as being intermediate in maturity, where thinking has coalesced around foundational paradigms which are continuing to be extended significantly.
5. The youngest areas are those at the longest time and space scales, all having something to do with devices: either discrete, or integrated into circuits and systems, and either static or evolving. Much of this work was published in the '90's. It can be viewed as being much less mature, where many of the foundational paradigms around which thinking might coalesce have not yet been created.



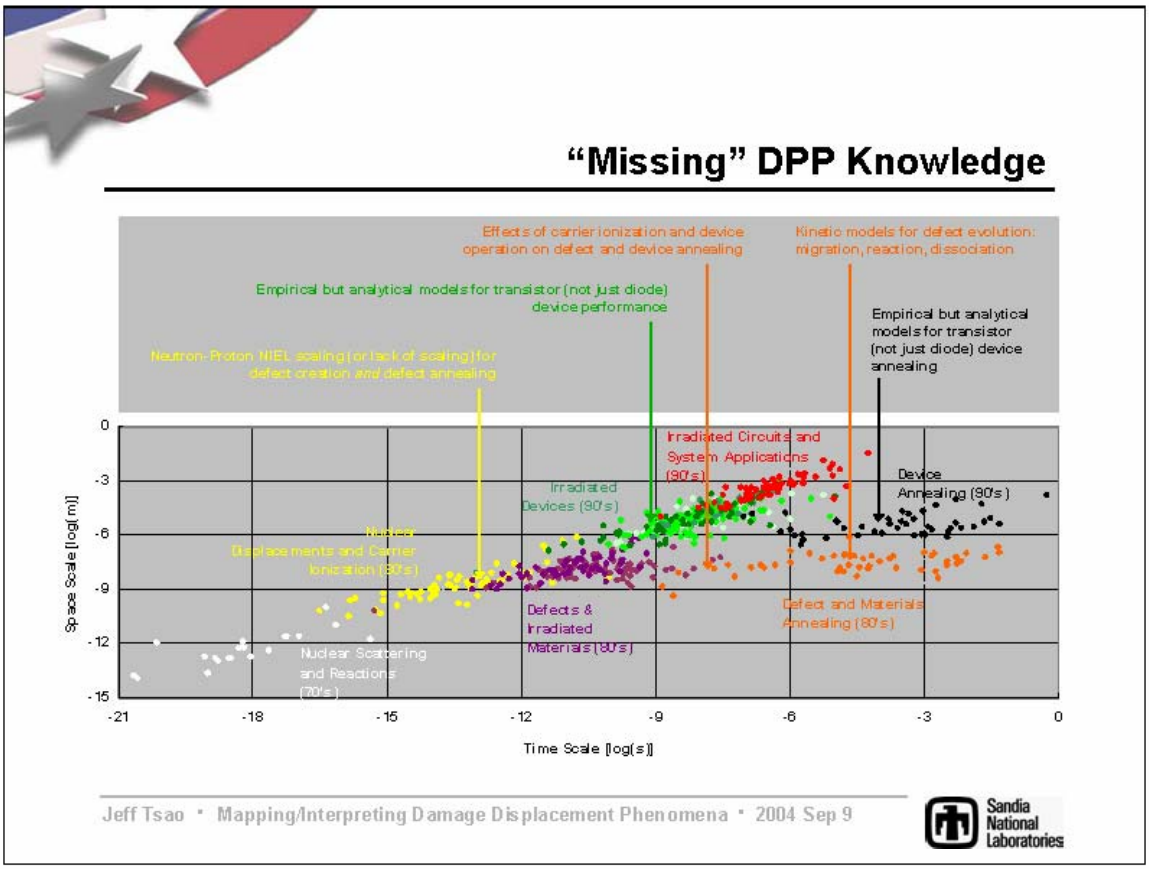
1. To see in more detail the kinds of knowledge that can be considered foundational to DPP phenomena, here we show on the map the six most cited articles in the database. All of them, not unexpectedly, are from the classes that can be considered more mature.
2. Three of them are have to do with nuclear displacements – the dynamics of the cascade of nuclear displacements that ultimately leads to point defects, clusters of point defects, and amorphous-like regions. The earliest two papers, from the 1950's, take an analytic approach to the problem. The more recent paper, from the 1970's, took a computer-simulation approach to the problem, and ultimately formed the basis for a now-well-known ion-implantation Monte Carlo computer-simulation code by UT Austin called Marlowe.
3. Two of them have to do with lattice defects – how to measure their electronic properties, and how those electronic properties affect device performance. The article by Lang introduced a technique called DLTS (deep-level transient spectroscopy) that revolutionized semiconductor defect characterization through its ability to quickly determine the energies and concentrations of defects which can trap charge. The article by Lax explained how charge trapping can be an extremely efficient process, and one can then anticipate that individual lattice defects can have a profound effect on device performance.
4. And, finally, one of them has to do with an analytical treatment of coupled transport and bimolecular reactions such as occurs during defect evolution.
5. Note that all of these articles represent the accumulation of knowledge and the creation of foundational paradigms at the lowest space scales. The accumulation of such knowledge and paradigms for understanding device phenomena, at a higher spatial scale, has been slower, but have been the subject of considerable interest in the 1990's and 2000's.



1. To see this, we can take a look at some "emerging" areas in the DPP knowledge domain. And, when we say "emerging" areas, we really mean two things. First, that the articles are highly cited; second, that they are recent.
2. The highly-cited part is, however, tricky, because we want to compare across articles published at different times. Hence, to make this comparison, we use a "projected citations" metric.
3. This metric is based on the idea that citations to articles accumulate roughly as a saturated exponential with time. Hence, if an article published in year y_o is in the long term ($y \rightarrow \infty$) going to have accumulated c_∞ citations, then in the year $y > y_o$ one can expect roughly $c = c_\infty(1-\exp\{-[(y-y_o)/\delta y]^\alpha\})$ citations, where δy is on the order 5-15 years, and the exponent α is on the order 1-2. This formula is plotted as the blue dashed line in the figure, for hypothetical articles published at various dates that will saturate at long times at 105 citations. In other words, the blue dashed curve is an iso-projected-citations contour for 105 citations.
4. We also show the citation statistics for all 650 or so of the articles in the database. Articles that are above this blue dashed line are projected to accumulate more than 105 citations over their lifetime, and the degree to which they are above this line indicates the degree to which they are projected to accumulate more than 105 citations.
5. Emerging areas of DPP knowledge can then be inferred to be those recent articles which, based on recent citation history, are *projected* to have large accumulated citations at long times. For our purpose, we use the area inside the dashed box -- the zone within which articles were published in 1990 or later, and are projected to accumulate more than 105 cites. There are six such articles.



1. These six articles are indicated on the space-time DPP map. These are the six articles from the 1990's and 2000's that have the most projected cites in the database.
2. There are still three articles treating small-spatial-scale aspects of the problem, indicating that there is still an active development of additional knowledge and paradigm extension in these aspects.
    1. The article by Nordlund and co-workers describes a much more sophisticated computer simulation technique, based on molecular dynamics, rather than Monte Carlo, techniques, for calculating defect production. These techniques are capable of describing in much more detail the types and distribution of defects. This kind of detailed knowledge is necessary to understand the evolution and reaction of those defects that occurs in the annealing step.
    2. The article by Summers and co-workers discusses the key issue of so-called NIEL scaling. The idea is that it is only the non-ionizing energy loss of an incident particle that enters into the production of lattice defects. Although within one particle type, this has been well-established, there is still controversy across particle types – i.e., in comparing electrons with protons, or protons with neutrons. If the scaling were perfect, then one could predict the effects of neutron exposure on a device, through tests made using proton exposure. But the scaling is evidently not perfect, probably because the details of the nuclear scattering and displacements are different, and hence the resulting defect distributions are different.
    3. The article by Corbett and co-workers describes a particular kind of defect, a divcancy, which is very common product of a vacancy-vacancy reaction in the lattice. This defect, which is no more complex than others that are also common, has a range of possible structures, hence a range of possible energy levels and effects on device performance. The structures that may be accessed depend on temperature, and hence device performance will depend on temperature.
3. But, in the 1990's, much activity emerged at a higher level of spatial aggregation: in the area of device performance. This was driven, in particular, by the emerging importance of silicon particle detectors for high-energy physics experiments. Three of the articles, all from the late 1990's or early 2000's, discuss progress in this area. They describe analytic models for device performance as a function of particle dose and annealing conditions. However, the models are still fairly empirical, and, although the attempt was made, do not yet incorporate a detailed connection to the underlying microscopic defects.



1. Finally, it may be interesting to see, from the perspective of the various classes on this map, what pieces of knowledge are yet missing that would enable the clusters to be connected, and hence to enable a "reductionist" and bottoms-up understanding of damage-displacement phenomena in Si junction devices. Here we give a list of four (more can probably be found):
2. First is the question of NIEL scaling. Is there some scaling relationship that allows cross-fertilization of data between neutron and proton irradiation experiments? This is of course a big deal because proton irradiation facilities are much less expensive than neutron irradiation facilities. The question is a complex one, because it involves not just the static "before and after" look at damage, but also the way in which the damage anneals. Even if static damage obeys a scaling relationship, there is no guarantee that damage annealing will.
3. Second is the question of the effects of carrier ionization and device operation on defect and device annealing. This question is related to the first, since there is the possibility that some annealing will occur during irradiation, in the presence of carriers created from the ionizing energy loss component of energy loss. But this question also extends our understanding to a new domain – annealing in the presence of device operation, and in the presence of device-operation-created carriers.
4. Third is the question of models not just for the influence of various kinds of defects on device performance, but for how the defects evolve – their migration, reaction, dissociation, subsequent migration, etc. The key issue is whether this migration, up until now treated more-or-less on a phenomenological basis, can be put on a more quantitative basis through detailed analysis of defect migration and reaction energetics.
5. Fourth and fifth are the questions of empirical but analytical models for transistor device performance and annealing. The high-energy physics community has done a thorough job of developing such models for diodes, resulting in the so-called "Hamburg" model for the performance and annealing of damaged devices. It was these models that enabled operational projections, within large error bars, of course) to be made. The key issues is whether similar models can be developed for transistor devices; thereby enabling similar operational projections, again within large error bars, to be made.

Distribution

1	MS 1167	K. M. Horn, 15343
1	MS 0114	N. M. Rahal, 5925
1	MS 0310	K. W. Boyack, 9212
1	MS 1081	C. E. Hembree, 1739
1	MS 0310	H. P. Hjalmarson, 9235
1	MS 0601	J. Y. Tsao, 1123
1	MS 1206	C. C. Mitchell, 5932
1	MS 1202	T. J. Drummond, 5917
1	MS 1056	S. M. Myers, 1112
1	MS 1415	J. C. Barbour, 1110
1	MS 0601	M. E. Coltrin, 1123
1	MS 0601	J. A. Simmons, 1120
1	MS 1427	J. M. Phillips, 1100
1	MS 0123	H. R. Westrich, 1011
1	MS 0511	W.B. Gauster, 1010
1	MS 9018	Central Technical Files, 8945-1
2	MS 0899	Technical Library, 9616
1	MS 0161	Patent and Licensing Office, 1150